

Supplementary Materials

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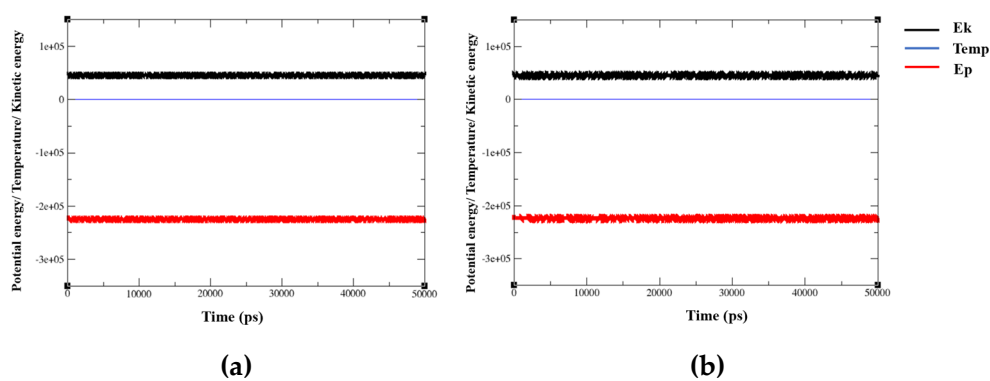


Figure S1. Kinetic, potential energy variations and temperature changes in the MD simulations of BVM (a) and DSC (b).

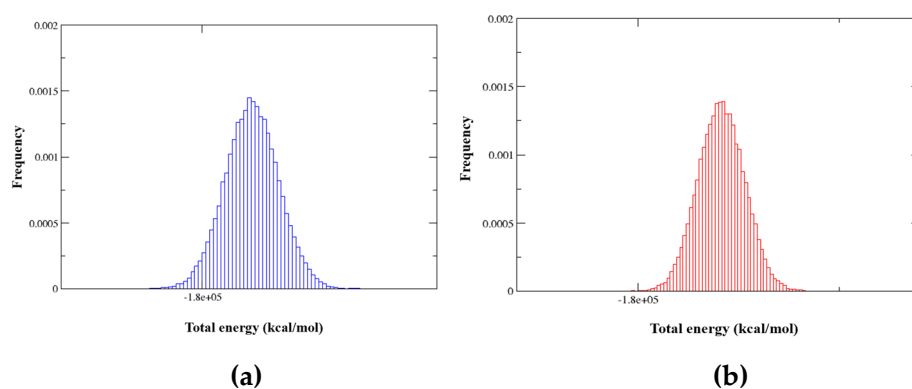


Figure S2. Total energy frequency distribution of BVM (a) and DSC (b).

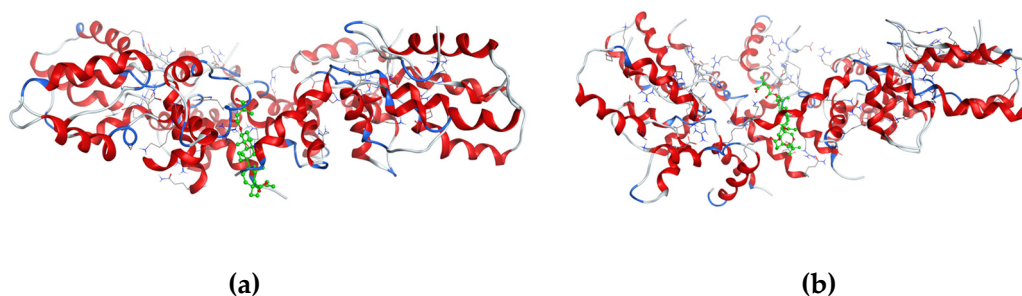


Figure S3. Lowest potential energy structure of BVM (a) and DSC (b). The graph represented the conformation with the lowest potential energy during the MDs process, which was equivalent to the most stable conformation of the molecule and had the highest probability of occurrence in the system.

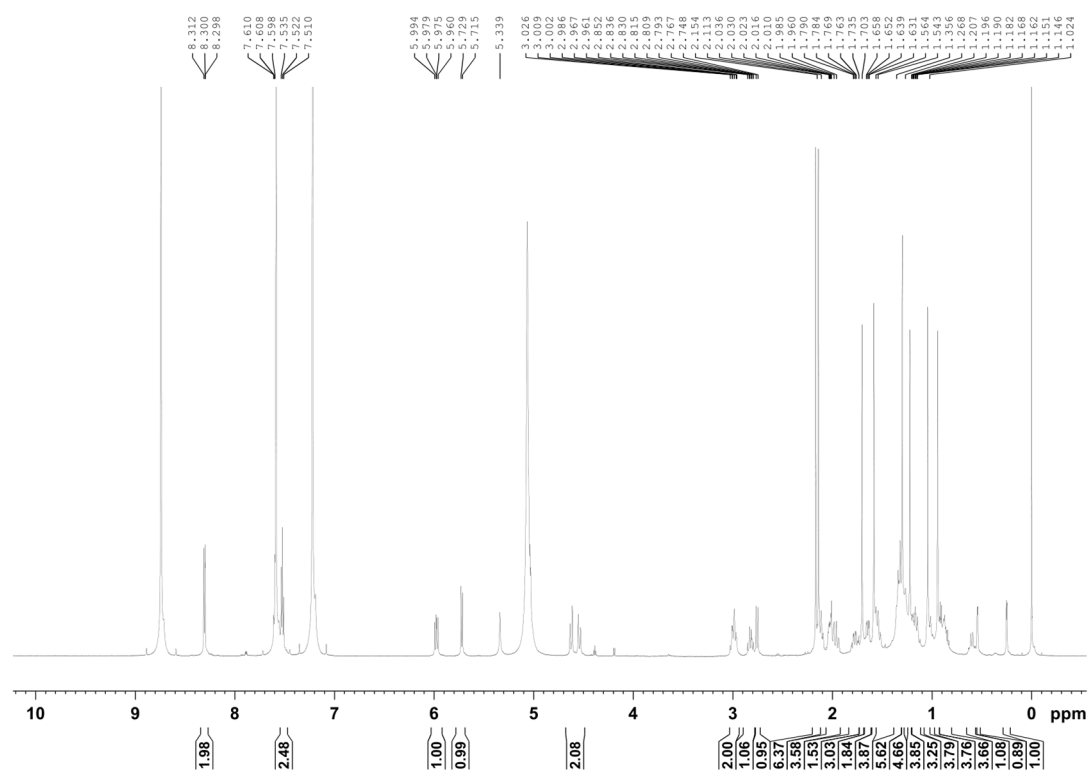


Figure S4. The ^1H NMR (600 MHz, pyridine-d_5) spectrum of the new derivative **2a**

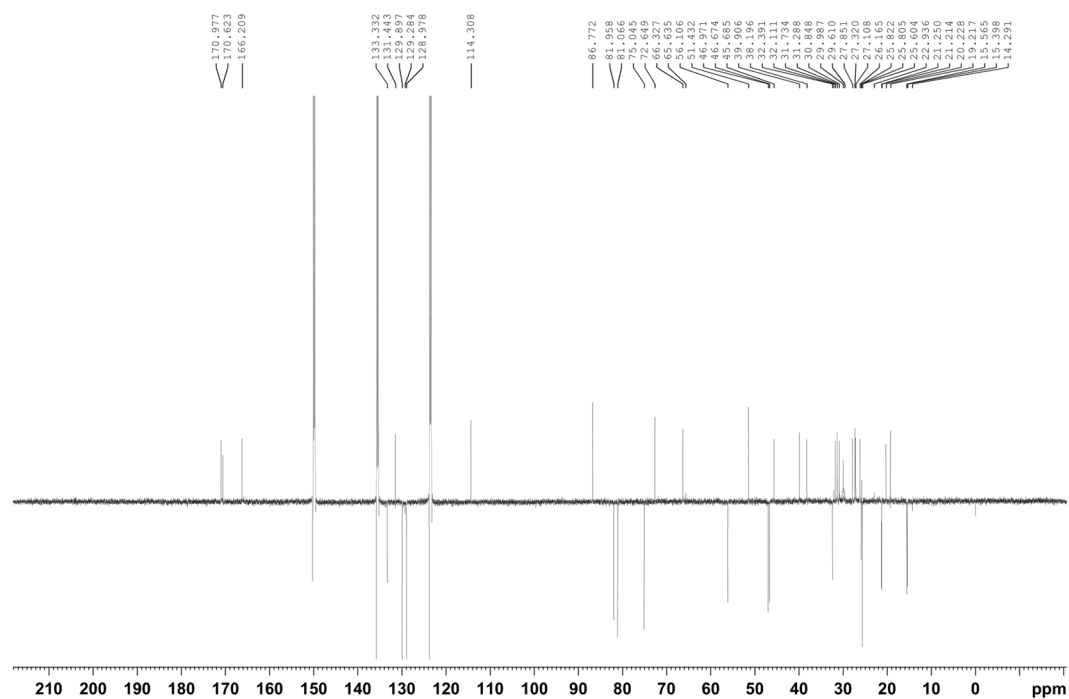


Figure S5. The ^{13}C NMR (150 MHz, pyridine- d_5) spectrum of the new derivative **2a**

BC-FTMS_220325142301#1 RT: 0.00 AV: 1 NL: 8.45E6
T: FTMS +pESI Full ms [50.00-2000.00]

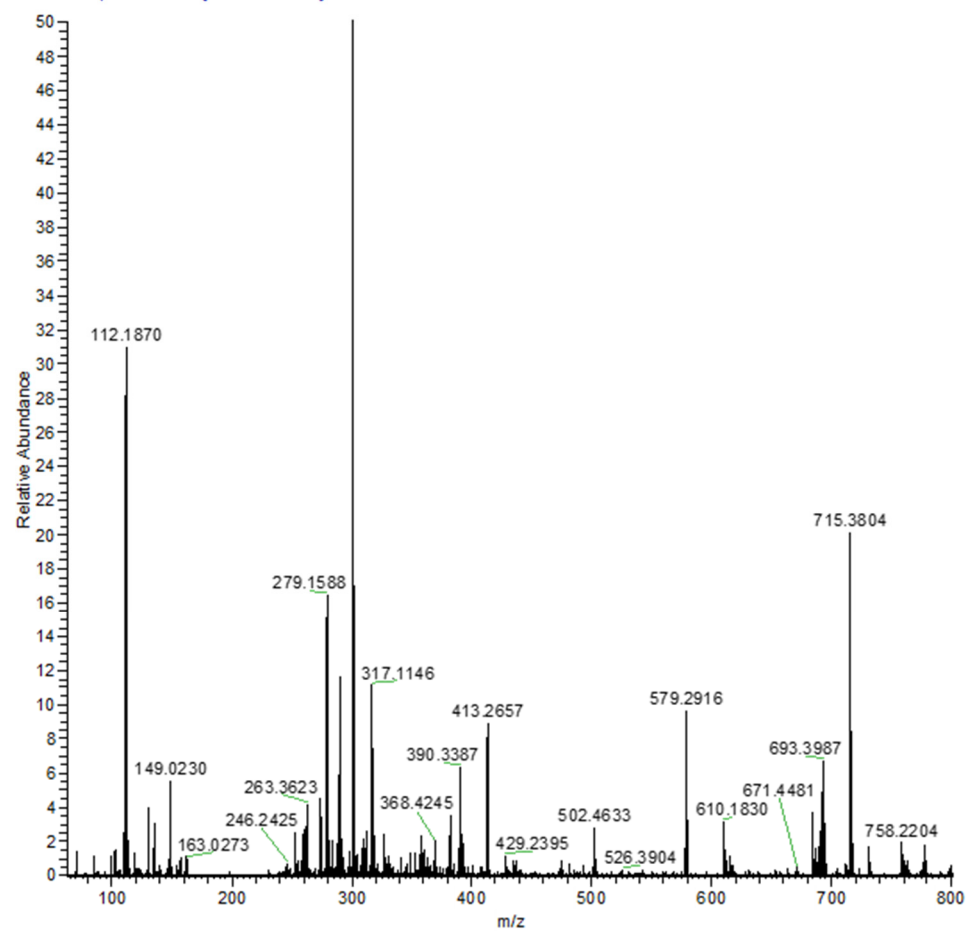


Figure S6. The HRESIMS spectrum of the new derivative **2a**

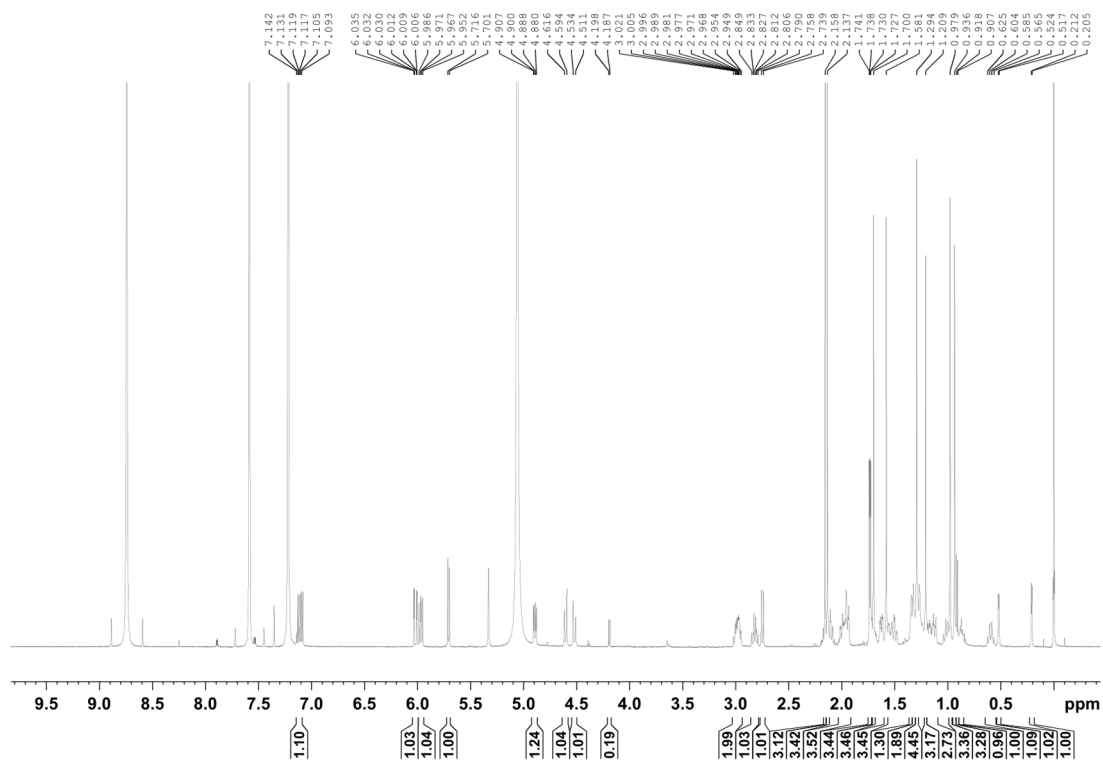


Figure S7. The ^1H NMR (600 MHz, pyridine- d_5) spectrum of the new derivative **2b**

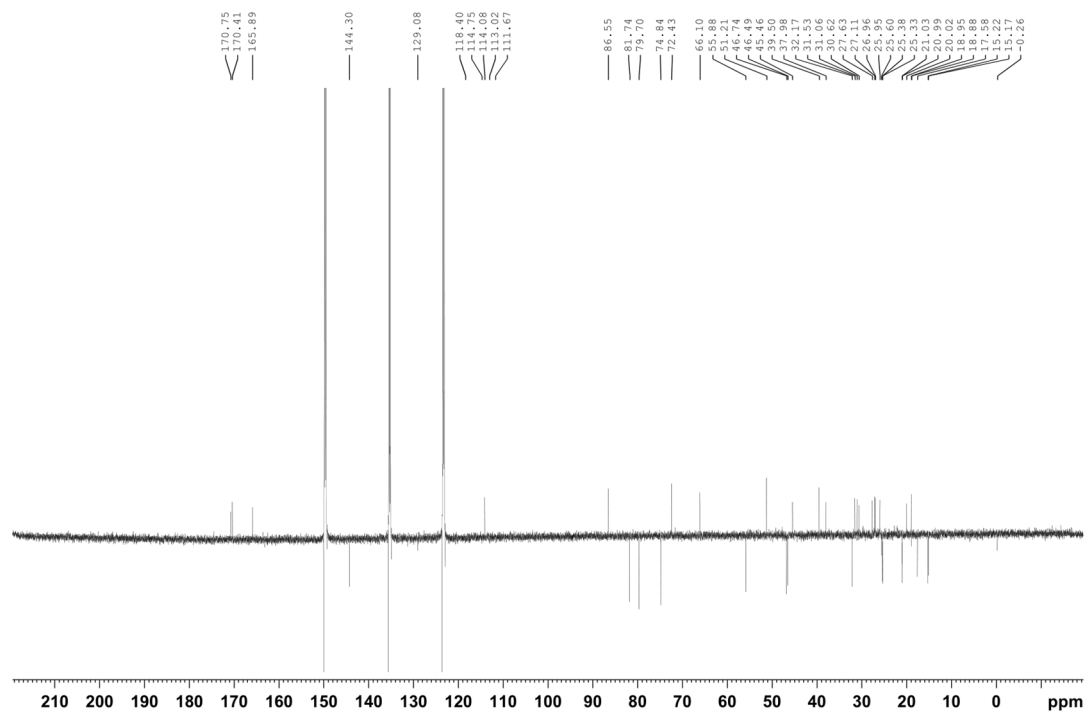


Figure S8. The ^{13}C NMR (150 MHz, pyridine- d_5) spectrum of the new derivative **2b**

CA-FTMS_220325142301#2 RT: 0.01 AV: 1 NL: 1.99E6
T: FTMS +p ESI Full ms [50.00-2000.00]

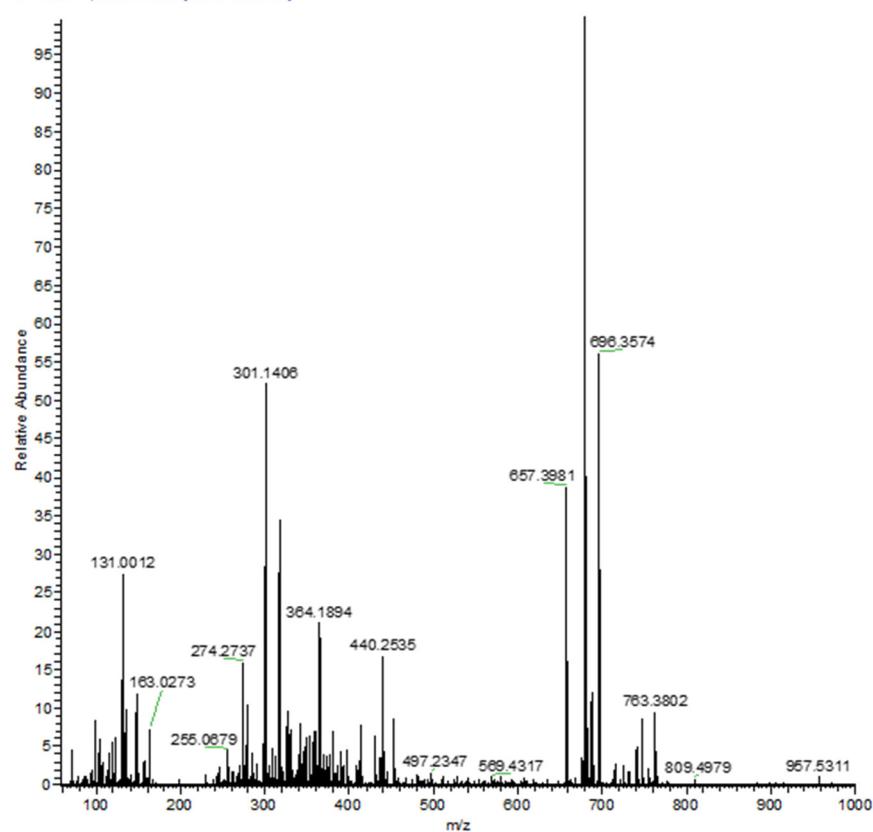


Figure S9. The HRESIMS spectrum of the new derivative **2b**

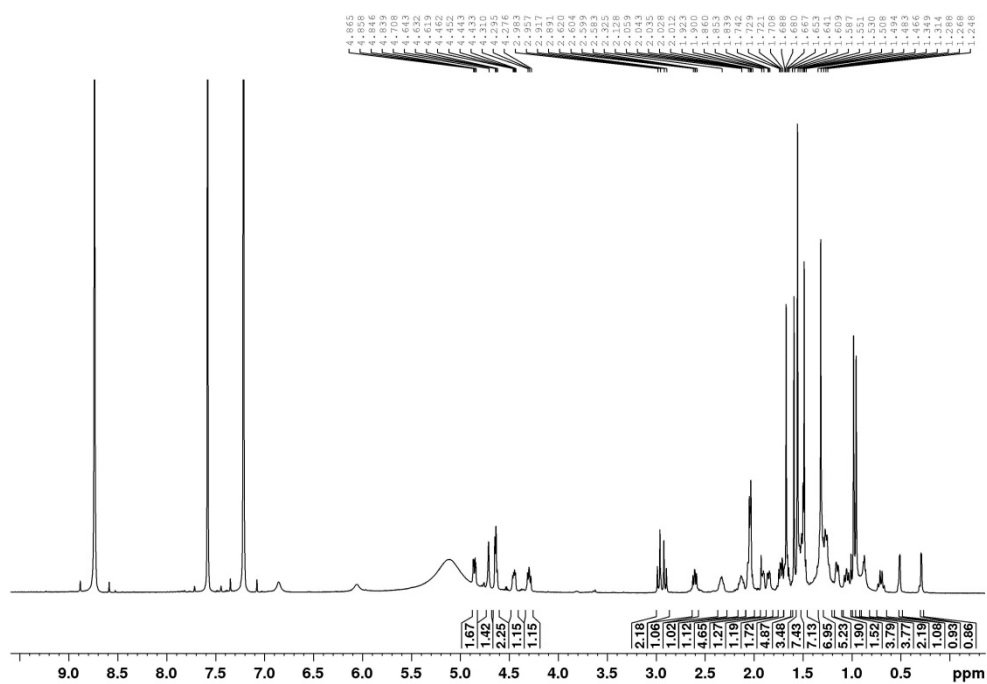


Figure S10. The ^1H NMR (600 MHz, $\text{pyridine-}d_5$) spectrum of the new derivative 3a



8_FTMS_20210512_210512145827 #11 RT: 0.09 AV: 1 NL: 5.60E6
T: FTMS + p ESI Full ms [200.00-1500.00]

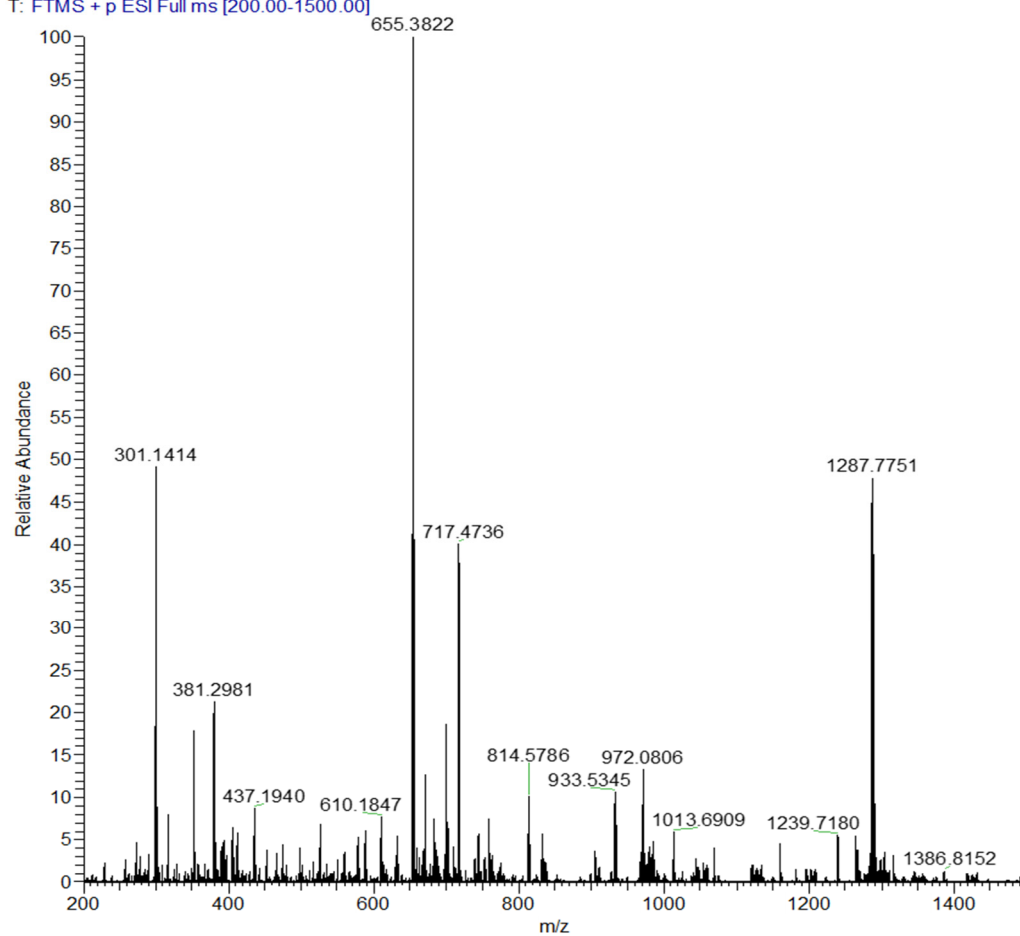
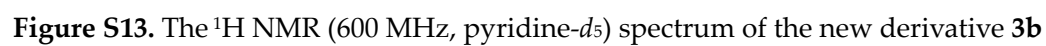


Figure S12. The HRESIMS spectrum of the new derivative **3a**



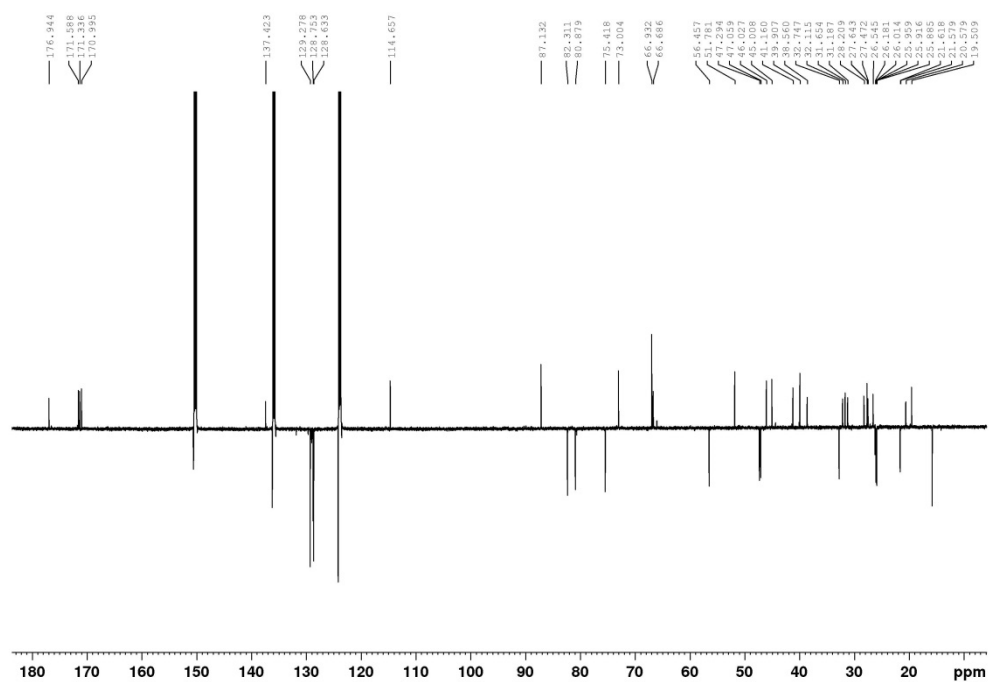


Figure S14. The ^{13}C NMR (150 MHz, pyridine- d_5) spectrum of the new derivative **3b**

9_FTMS_20210512_210512145827 #3 RT: 0.02 AV: 1 NL: 1.24E7
T: FTMS + p ESI Full ms [200.00-1500.00]

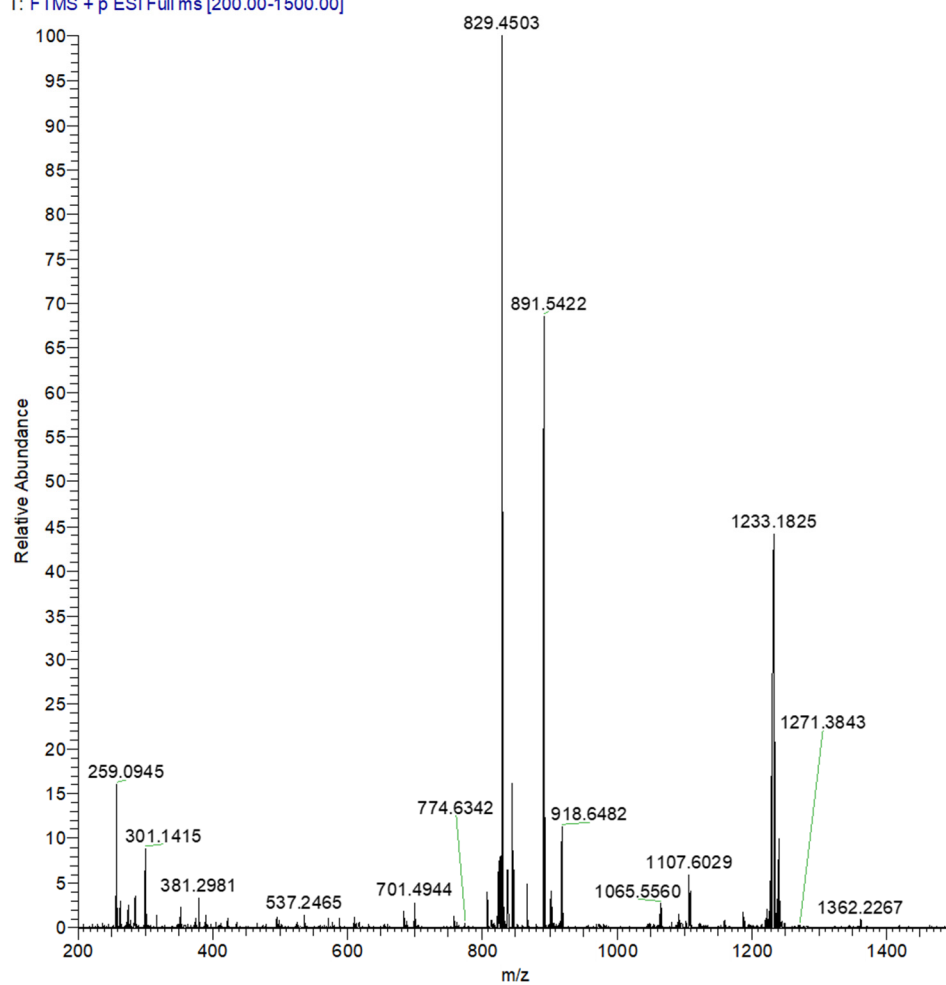


Figure S15. The HRESIMS spectrum of the new derivative **3b**

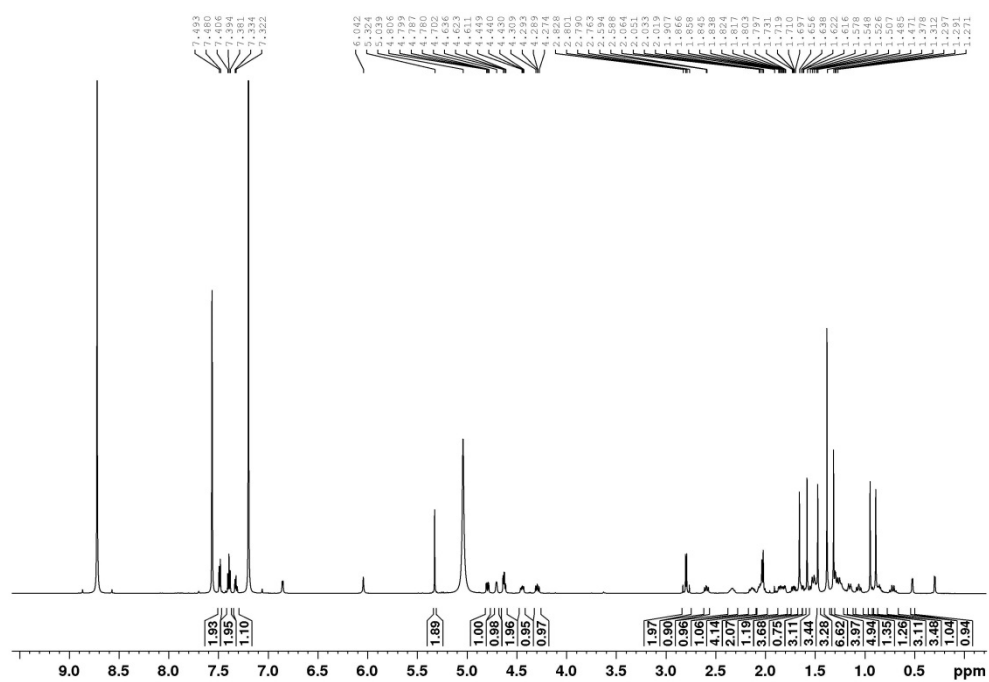


Figure S16. The ^1H NMR (600 MHz, $\text{pyridine-}d_5$) spectrum of the new derivative 3c

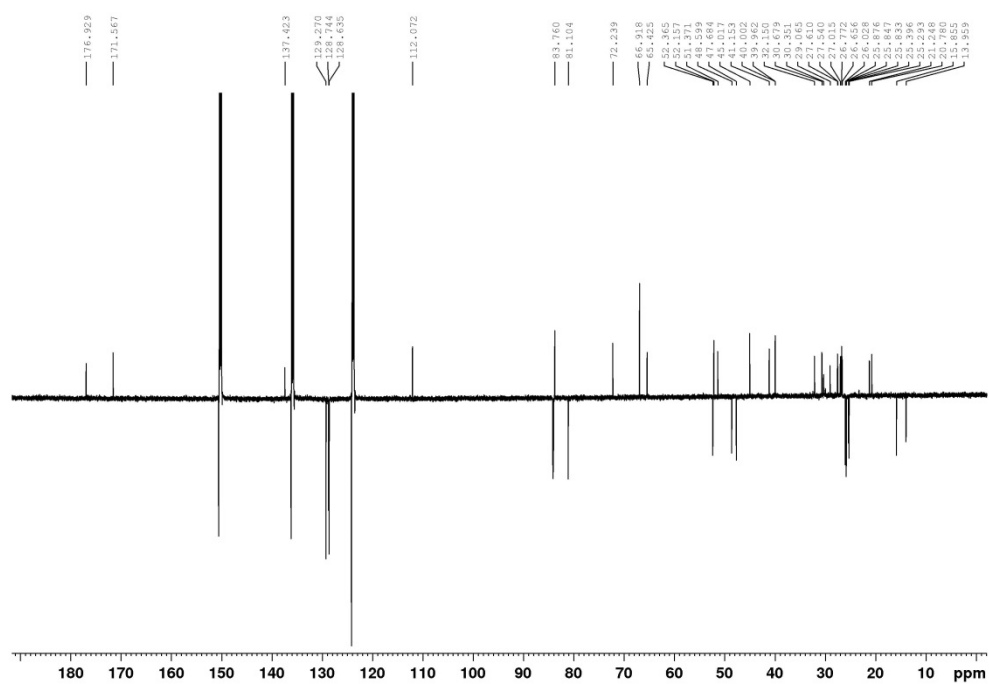


Figure S17. The ^{13}C NMR (150 MHz, pyridine- d_5) spectrum of the new derivative **3c**

10_FTMS_20210512_210513104007 #10 RT: 0.08 AV: 1 NL: 3.06E6
T: FTMS +p ESI Full ms [200.00-1500.00]

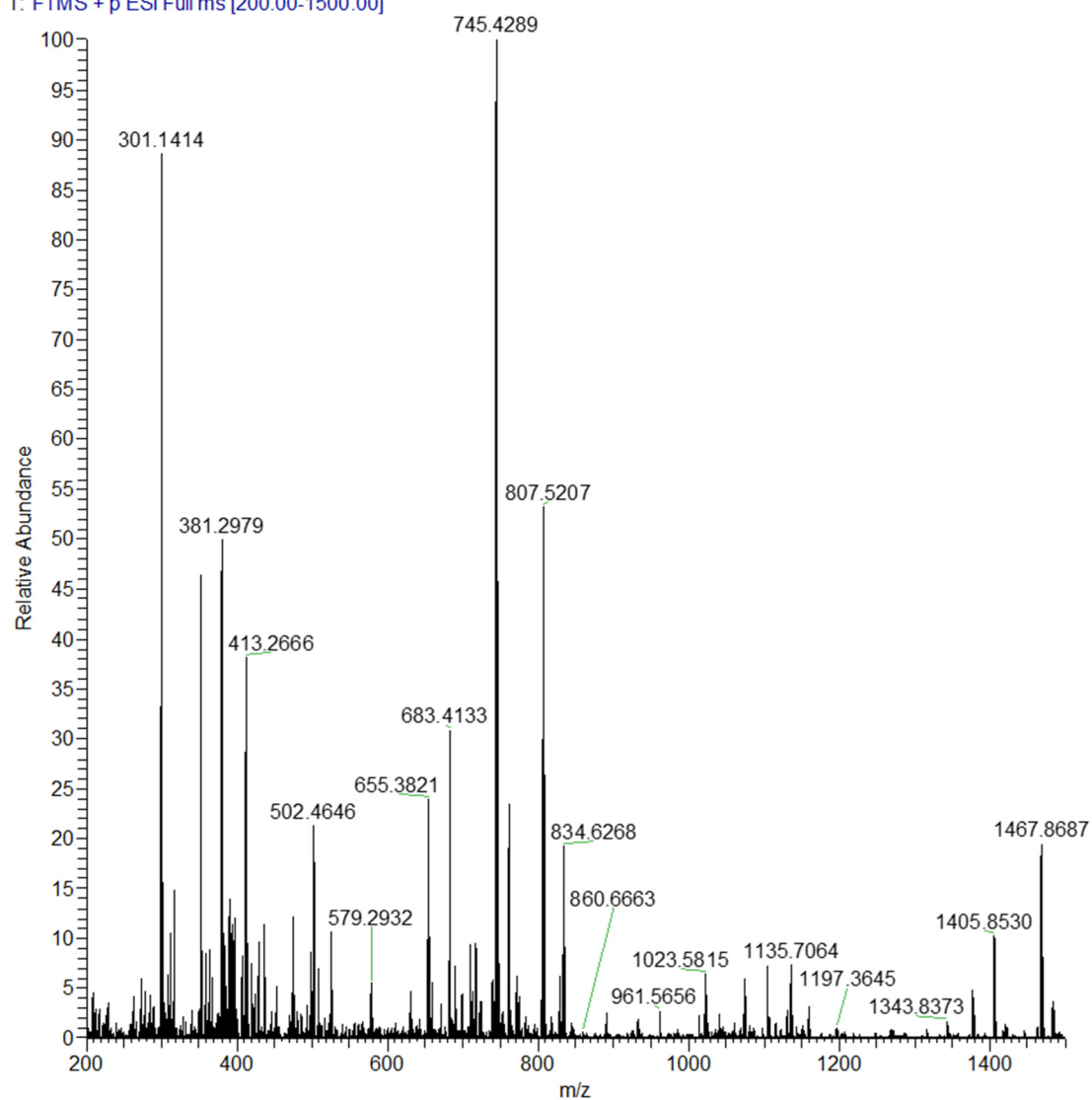


Figure S18. The HRESIMS spectrum of the new derivative **3c**